

Perturbative Heavy Quark Fragmentation Function through $\mathcal{O}(\alpha_s^2)$

Kirill Melnikov and Alexander Mitov

*Department of Physics and Astronomy,
University of Hawaii,
Honolulu, HI, 96822*

We derive the initial condition for the perturbative fragmentation function of a heavy quark through order $\mathcal{O}(\alpha_s^2)$ in the $\overline{\text{MS}}$ scheme. This initial condition is useful for computing heavy quark (or lepton, in case of QED) energy distributions from calculations with massless partons. In addition, the initial condition at $\mathcal{O}(\alpha_s^2)$ can be used to resum collinear logarithms $\ln(Q^2/m^2)$ in heavy quark energy spectrum with next-to-next-to-leading logarithmic accuracy by solving the DGLAP equation.

I. INTRODUCTION

Production of heavy flavors (charm and bottom) in high energy processes has become an important subject in the last decade, due to experiments at e^+e^- and hadron colliders. Since the center of mass energy of these machines is much larger than bottom and charm quark masses, it is tempting to consider such processes in the massless approximation. Unfortunately, this is only possible for sufficiently inclusive observables, for example, total cross-sections. However, differential distributions are more relevant for experimental analysis and, in addition, contain more information about the underlying physics. An interesting example is the energy distribution of heavy hadrons produced in a high-energy collision, since it gives direct access to the hadronization process. In perturbation theory, however, the heavy quark energy distribution diverges in the limit $m \rightarrow 0$ and the sensitivity to the quark mass m remains at arbitrary high energies.

This sensitivity is disagreeable for two reasons. First, it implies that energy spectra must be computed retaining quark masses which makes the calculations quite involved. Second, in higher orders of perturbation theory, energy spectra contain powers of logarithms $\ln(Q^2/m^2)$, that may invalidate fixed order perturbative calculations.

Both of these problems are solved by introducing perturbative fragmentation function [1]. This function describes the probability that a massless parton of a certain type fragments into a heavy quark. The mass of the heavy quark provides a natural cut-off for the collinear radiation, thus making perturbative predictions finite. The perturbative fragmentation function satisfies the DGLAP evolution equation [2]. By solving this equation, we can sum up large collinear logarithms $\ln(Q^2/m^2)$ that appear in perturbative fragmentation function and improve the quality of perturbative calculations. To avoid confusion, we note that a meaningful prediction for heavy hadron energy spectrum can only be obtained if the heavy quark energy distribution is convoluted with a non-perturbative fragmentation function. Such functions are traditionally extracted by fitting hadron energy spectra in e^+e^- collisions. We will not discuss this issue here; for recent work on the subject see [3]. We also note that the concept of perturbative fragmentation is useful outside QCD; for example, QED effects in the electron energy spectrum in muon decay, currently under study by the TWIST collaboration [4], can be analyzed using the same technique [5].

Because the Q^2 evolution of the fragmentation function can be obtained from the DGLAP equation, the perturbative fragmentation function at arbitrary Q^2 can be fully reconstructed once the initial condition D^{ini} and the time-like splitting kernels for the DGLAP evolution are known. The initial condition is usually computed at $Q^2 \sim m^2$; this ensures that no large logarithms appear and fixed order perturbation theory is reliable.

The purpose of this paper is to provide such initial condition for the perturbative fragmentation function through $\mathcal{O}(\alpha_s^2)$. As we explained earlier, the knowledge of D^{ini} through next-to-next-to-leading order (NNLO) enables the calculation of energy spectra of heavy quarks through $\mathcal{O}(\alpha_s^2)$ from massless results and, simultaneously, allows to resum large logarithms $\ln(Q^2/m^2)$ using the DGLAP equation. All power corrections $\mathcal{O}(m^2/Q^2)$ are neglected within this approach, but for many practical purposes such precision is sufficient.

Technically, the use of perturbative fragmentation functions makes it possible to compute the heavy quark energy spectrum in two steps – we first compute the energy spectrum of massless partons produced in a hard scattering and then convolute this spectrum with perturbative fragmentation function. The possibility to remove all the dependence on the heavy quark mass from the calculation of the hard scattering simplifies the computations considerably.

The remainder of the paper is organized as follows. In Section II we describe the process-independent derivation of the initial condition for the fragmentation function. Then, we discuss collinear factorization when finite quark masses are present and explain how to compute D^{ini} from relevant Feynman diagrams. We also suggest a suitable modification of the original proposal [6, 7] for the process-independent computation of the initial condition; such modification significantly simplifies NNLO calculations. In Section IV the initial condition for the fragmentation function for both quark- and gluon-initiated processes is computed through NLO. This computation allows us to demonstrate the details of our approach and to derive the NLO perturbative fragmentation function through $\mathcal{O}(\epsilon)$, where ϵ is the dimensional regularization parameter. In Section V we describe the calculation of the $\mathcal{O}(\alpha_s^2)$ contribution to the fragmentation function and present the result for the initial condition. We conclude in Section VI.

II. PROCESS-INDEPENDENT DERIVATION OF D^{ini}

Consider production of a heavy quark \mathcal{Q} with mass m and a definite value of energy $E_{\mathcal{Q}}$ in a hard scattering process. According to the QCD factorization theorems [8, 9, 10], the heavy quark energy spectrum can be computed as a convolution of the energy distribution of massless partons produced in the hard process, and the fragmentation function that describes the probability that the massless parton fragments into a massive quark with a definite energy. If the energy fraction $E_{\mathcal{Q}}/E_{\mathcal{Q},\text{max}}$ of the heavy quark is denoted by z , then the energy distribution of that quark can be written as:

$$\frac{d\sigma_{\mathcal{Q}}}{dz}(z, Q, m) = \sum_a \int_z^1 \frac{dx}{x} \frac{d\hat{\sigma}_a}{dx}(x, Q, \mu) D_{a/\mathcal{Q}}\left(\frac{z}{x}, \frac{\mu}{m}\right). \quad (1)$$

Here the sum runs over all partons (quarks, antiquarks and gluons) that can be produced in the hard process and μ is the factorization scale. The coefficient function $d\hat{\sigma}_a/dx$ is the $\overline{\text{MS}}$ renormalized differential cross-section for producing a massless parton a ¹. It is defined indirectly through the equation

$$\frac{d\sigma_a}{dz}(z, Q, \epsilon) = \sum_b \frac{d\hat{\sigma}_b}{dz}(z, Q, \mu) \otimes \Gamma_{ba}(z, \mu, \epsilon), \quad (2)$$

where $d\sigma_a/dz$ is the bare energy distribution for the parton of type a ; the collinear divergences in this distribution are regularized by working in $d = 4 - 2\epsilon$ dimensions. Γ_{ab} are universal collinear subtraction terms, defined in the $\overline{\text{MS}}$ scheme:

$$\Gamma_{ba} = \delta_{ab}\delta(1-z) - \left(\frac{\alpha_s}{2\pi}\right) \frac{P_{ab}^{(0)}(z)}{\epsilon} + \left(\frac{\alpha_s}{2\pi}\right)^2 \left[\frac{1}{2\epsilon^2} \left(P_{ac}^{(0)} \otimes P_{cb}^{(0)}(z) + \beta_0 P_{ab}^{(0)}(z) \right) - \frac{1}{2\epsilon} P_{ab}^{(1)}(z) \right], \quad (3)$$

where $\alpha_s = \alpha_s(\mu)$ is the $\overline{\text{MS}}$ strong coupling constant, renormalized at the scale μ . The relation between the bare and the renormalized couplings reads:

$$\frac{\alpha_s^0}{2\pi} S_\epsilon = \frac{\alpha_s}{2\pi} \left(1 - \frac{\alpha_s}{2\pi} \frac{\beta_0}{\epsilon} + \mathcal{O}(\alpha_s^2) \right), \quad (4)$$

where $S_\epsilon = (4\pi)^\epsilon e^{-\epsilon\gamma}$ and γ is the Euler constant. Also, $\beta_0 = (11C_A - 4T_R n_f)/6$ is the $\mathcal{O}(\alpha_s^2)$ coefficient of the QCD β -function, $C_A = 3$, $T_R = 1/2$ are the QCD color factors, n_f denotes the number of fermion flavors (including \mathcal{Q}) and $P_{ab}^{(0,1)}$ are the time-like splitting functions [11]. Our notations for the splitting functions follow Ref.[10].

The functions $D_{a/\mathcal{Q}}(x, \mu/m)$ in Eq.(1) are the perturbative fragmentation functions [1]. They satisfy the DGLAP evolution equation and can be fully reconstructed from it, if the initial condition at a scale $\mu = \mu_0$ is known. We denote

$$D_{a/\mathcal{Q}}\left(z, \frac{\mu_0}{m}\right) = D_a^{\text{ini}}\left(z, \frac{\mu_0}{m}\right). \quad (5)$$

¹ In the evaluation of the coefficient function $d\hat{\sigma}_a/dx$ the heavy quark \mathcal{Q} is considered as massless; therefore, the sum over indexes in Eq.(1) includes the flavor \mathcal{Q} .

If $\mu_0 \sim m$ is chosen, the initial condition D_a^{ini} does not contain large logarithms and can be derived from fixed order perturbative calculations. Setting $\mu = \mu_0$ in Eq.(1), we obtain:

$$\frac{d\sigma_{\mathcal{Q}}^{\text{fo}}}{dz}(z, Q, m) = \sum_a \frac{d\hat{\sigma}_a}{dz}(z, Q, \mu_0) \otimes D_a^{\text{ini}}\left(z, \frac{\mu_0}{m}\right), \quad (6)$$

where $d\sigma^{\text{fo}}$ is the fixed order cross-section for producing a quark \mathcal{Q} with mass m , with all power corrections $\mathcal{O}((m^2/Q^2)^n)$, $n \geq 1$ systematically neglected. It follows from this equation that the initial condition for the fragmentation function can be extracted, if the heavy quark energy spectrum is computed in a particular process through certain order in α_s . This, however, is technically inconvenient.

A more convenient, process-independent approach was suggested recently in Refs.[6, 7]. Since hard scattering cross-sections are insensitive to long-distance dynamics, we may write

$$\frac{d\sigma_{\mathcal{Q}}^{\text{fo}}}{dz}(z, Q, m) = \sum_a \frac{d\tilde{\sigma}_a}{dz}(z, Q, \mu_0) \otimes \tilde{D}_{a/\mathcal{Q}}\left(z, \frac{\mu_0}{m}\right), \quad (7)$$

$$\frac{d\sigma_b}{dz}(z, Q, \epsilon) = \sum_a \frac{d\tilde{\sigma}_a}{dz}(z, Q, \mu_0) \otimes \tilde{D}_{a/b}^L(z, \mu_0, \epsilon). \quad (8)$$

The functions \tilde{D} and \tilde{D}^L describe collinear radiation from massive (massless) quarks; we will show below that they can be considered as bare fragmentation functions. Combining Eqs.(7,8) with Eqs.(6,2), we obtain:

$$\tilde{D}_{a/\mathcal{Q}}\left(z, \frac{\mu_0}{m}\right) = \sum_{b,c} \tilde{D}_{a/b}^L(z, \mu_0, \epsilon) \otimes [\Gamma(z, \mu_0, \epsilon)]_{bc}^{-1} \otimes D_c^{\text{ini}}\left(z, \frac{\mu_0}{m}\right). \quad (9)$$

It follows from this equation that D^{ini} can be derived once \tilde{D} and \tilde{D}^L are known. We describe how to compute \tilde{D} and \tilde{D}^L in the next Section.

To conclude this Section, we comment on the analytic structure of D^{ini} . The initial condition for the perturbative fragmentation function can be expanded in series of α_s :

$$D_a^{\text{ini}}\left(z, \frac{\mu_0}{m}\right) = \sum_{n=0} \left(\frac{\alpha_s(\mu_0)}{2\pi}\right)^n d_a^{(n)}\left(z, \frac{\mu_0}{m}\right). \quad (10)$$

The results through $\mathcal{O}(\alpha_s)$ are known [1]:

$$\begin{aligned} d_a^{(0)}(z) &= \delta_{a\mathcal{Q}}\delta(1-z), \\ d_{a=\mathcal{Q}}^{(1)}\left(z, \frac{\mu_0}{m}\right) &= C_F \left[\frac{1+z^2}{1-z} \left(\ln\left(\frac{\mu_0^2}{m^2(1-z)^2}\right) - 1 \right) \right]_+, \\ d_{a=g}^{(1)}\left(z, \frac{\mu_0}{m}\right) &= T_R (z^2 + (1-z)^2) \ln\left(\frac{\mu_0^2}{m^2}\right), \\ d_{a \neq \mathcal{Q}, g}^{(1)}\left(z, \frac{\mu_0}{m}\right) &= 0, \end{aligned} \quad (11)$$

where $C_F = 4/3$ is the QCD color factor. In this paper, we are mostly concerned with the computation of the coefficients $d_{\mathcal{Q}, \bar{\mathcal{Q}}, q, \bar{q}}^{(2)}$, where q stands for any massless quark. The logarithmically enhanced terms in $d^{(2)}$ follow from the DGLAP equation:

$$\begin{aligned} d_a^{(2)}\left(z, \frac{\mu_0}{m}\right) &= \left[\frac{P_{ba}^{(0)} \otimes P_{\mathcal{Q}b}^{(0)}(z)}{2} + \frac{\beta_0}{2} P_{\mathcal{Q}a}^{(0)}(z) \right] \ln^2\left(\frac{\mu_0^2}{m^2}\right) \\ &+ \left[P_{\mathcal{Q}a}^{(1)}(z) + P_{ba}^{(0)} \otimes d_b^{(1)}(z, 1) + \beta_0 d_a^{(1)}(z, 1) \right] \ln\left(\frac{\mu_0^2}{m^2}\right) + d_a^{(2)}(z, 1). \end{aligned} \quad (12)$$

The mass-independent constant of integration $d_a^{(2)}(z, 1)$ can not be determined from the DGLAP equation and has to be computed explicitly. This is the major goal of this paper. In the next Section we describe how this can be done.

III. THE COLLINEAR LIMIT

The idea that allows explicit computation of the functions \tilde{D}^L and \tilde{D} and, therefore, of the initial condition for the perturbative fragmentation function is as follows. Both \tilde{D} and \tilde{D}^L are introduced to describe collinear radiation with $q_\perp \sim m \leq \mu_0$. Since we are not interested in power-suppressed contributions to the cross-section, we can restrict ourselves to such terms in scattering amplitudes that, upon integration over the phase-space of final state particles, produce $\mathcal{O}(\ln^n(m))$, $n \geq 1$ terms². Such terms can be identified by applying power counting arguments [9] in the collinear limit for scattering amplitudes. The collinear limit is defined as the kinematic limit where the relative transverse momentum of two or more particles vanishes. When masses are introduced, the collinear limit is $q_\perp \rightarrow 0$, $m \rightarrow 0$ and $q_\perp/m = \text{const}$ [12].

Throughout the paper we work in the light-cone gauge $n_\mu A^\mu = 0$, $n^2 = 0$. This is necessary for the process-independent derivation of D^{ini} because in such gauges, the $\mathcal{O}(\ln^n(m))$, $n \geq 1$ terms are produced only by diagrams where collinear radiation is both emitted and absorbed by the same parton. The quantum interference effects in such gauges can be integrated over the phase-space of the final state particles in the massless approximation. Because of that, D^{ini} can be computed from self-energy type diagrams, integrated over the virtuality of the incoming parton. Different cuts of such self-energy diagrams correspond to different contributions to the fragmentation function: at $\mathcal{O}(\alpha_s^2)$, we have to deal with two-loop virtual corrections, one-loop virtual corrections to one-to-two splittings and, finally, one-to-three splittings.

We begin by considering the one-to-three collinear splitting since the kinematics of the final state in this case is the most general. We denote the four-momenta of the produced (massive or massless) particles by $q_{1,2,3}$ and their sum by \hat{p} :

$$\hat{p} = q_1 + q_2 + q_3. \quad (13)$$

We parameterize the collinear direction by p and use the gauge fixing vector n as the complimentary light-cone vector. We then write:

$$q_i = z_i p + \beta_i \frac{n}{(pn)} + q_{i,\perp}. \quad (14)$$

The components β_i are found from the on-shell conditions $q_i^2 = m_i^2$:

$$\beta_i = \frac{-q_{i,\perp}^2 + m_i^2 - z_i^2 m_p^2}{2z_i}, \quad i = 1, 2, 3, \quad (15)$$

with $p^2 = m_p^2$. We are interested in the case when \hat{p}, p and n belong to the same hyperplane in the d -dimensional space³. Then:

$$z_1 + z_2 + z_3 = 1, \quad q_{1,\perp} + q_{2,\perp} + q_{3,\perp} = 0. \quad (16)$$

Using the above equations, we express the momentum \hat{p} through p and n :

$$\hat{p} = p + \frac{1}{2}(\hat{p}^2 - m_p^2) \frac{n}{(pn)}, \quad (17)$$

where:

$$\hat{p}^2 - m_p^2 = \frac{2(pq_2) + 2(pq_3) - 2(q_2q_3) + m_1^2 - m_2^2 - m_3^2 - m_p^2}{z}.$$

Our notations are such that q_1 always denotes the momentum of the heavy quark in the final state, whose energy is measured. For that reason we often write z instead of z_1 , to denote its energy fraction. Eqs.(14,16) imply the relation:

$$z = 1 - \frac{(nq_2)}{(pn)} - \frac{(nq_3)}{(pn)}, \quad (18)$$

² To be precise, we are interested in all contributions to the scattering amplitude that, upon integration over the phase space, scale as $m^{-n\epsilon}$, where n is some integer. Upon expanding in ϵ , those terms produce *both* $\ln(m)$ -enhanced and m -independent contributions to the energy spectrum.

³ More general configuration has been considered in [13].

which is nothing but the energy conservation condition.

Although we have only discussed the kinematics of the one-to-three splitting, the kinematics of the one-to-two splitting can be obtained as a particular case. For this, it is sufficient to set the momentum q_3 and the mass m_3 to zero in the equations above.

In QCD, factorization properties of the cross-sections, as in Eqs.(7,8), can be traced back to the factorization properties of both the phase-space and the matrix elements in the collinear kinematics. We illustrate those properties by considering the tree level amplitudes and then generalize these considerations to include virtual corrections.

Consider a hard scattering process characterized by some scale $Q \gg m$. Suppose that $n+2$ partons with momenta $k_1, \dots, k_{n-1}, q_1, q_2, q_3$ are produced. We consider momenta k_1, \dots, k_{n-1} as non-exceptional, while momenta q_1, q_2, q_3 are collinear, as described above. First, we discuss the phase-space factorization.

We denote the phase-space of $n+2$ partons as $\text{dPS}^{(n+2)}(k_1, \dots, k_{n-1}, q_1, q_2, q_3)$. In the limit when q_1, q_2 and q_3 become collinear $q_1 + q_2 + q_3 = p + \mathcal{O}(q_\perp)$, the $(n+2)$ -particle phase space factorizes:

$$\text{dPS}^{(n+2)}(k_1, \dots, k_{n-1}, q_1, q_2, q_3) = \text{dPS}^{(n)}(k_1, \dots, k_{n-1}, p) \text{d}\Phi^{\text{coll}}(q_2, q_3). \quad (19)$$

We use the following notations:

$$\text{d}\Phi^{\text{coll}}(q_2, q_3) = \frac{1}{z} [dq_2; m_2] [dq_3; m_3], \quad (20)$$

and $[dq; m_q]$ is the d -dimensional one-particle phase space:

$$[dq; m_q] = \frac{d^d q}{(2\pi)^{d-1}} \delta^+(q^2 - m_q^2). \quad (21)$$

To derive Eq.(19), we neglect the $\mathcal{O}(q_\perp, m)$ difference between \hat{p} and p in $\text{dPS}^{(n)}$ and integrate over q_1 using Eq.(13).

We now consider factorization properties of the tree-level matrix element. In the massless case, they were described in [13, 14]. Below we generalize those results to the case of non-zero mass m . We consider massive quarks produced in the fragmentation of a quark-like parton of either the same or different flavor. The case of a gluon fragmentation into a heavy quark can be dealt with in a similar way.

We already mentioned that, in physical gauges, the relevant contributions in the collinear limit come from diagrams where the same parton emits and absorbs collinear radiation. Taken in conjunction with power counting arguments, this observation can be used to simplify tree-level matrix elements in the collinear limit and derive the factorization formula. Consider a process with $n+2$ particles in the final state described by the matrix element $M^{(n+2)}(k_1, \dots, k_{n-1}, q_1, q_2, q_3)$. In physical gauges, the collinear splitting $\hat{p} \rightarrow q_1 + q_2 + q_3$ decouples from the rest of the process, so that the squared, spin-averaged amplitude $|M^{(n+2)}|^2$ can be written as [13]:

$$|M^{(n+2)}(k_1, \dots, k_{n-1}, q_1, q_2, q_3)|^2 = \mathcal{M}^{(n)}(k_1, \dots, k_{n-1}, \hat{p})_{\beta, \alpha} V_{\alpha, \beta}^{\text{coll}}(\hat{p}, q_2, q_3). \quad (22)$$

Here α, β are spinor indices. If, in the collinear limit, V^{coll} can be written as

$$V_{\alpha, \beta}^{\text{coll}} = \not{p}_{\alpha, \beta} W + \mathcal{O}(q_\perp), \quad (23)$$

we can rewrite Eq.(22) to make the factorization of the matrix element explicit:

$$|M^{(n+2)}(k_1, \dots, k_{n-1}, q_1, q_2, q_3)|^2 = |M^{(n)}(k_1, \dots, k_{n-1}, p)|^2 W(n, \hat{p}, q_2, q_3) + \mathcal{O}(q_\perp). \quad (24)$$

Here $|M^{(n)}(\dots, p)|^2$ is the amplitude squared for producing n on-shell particles with non-exceptional momenta; the scalar function W contains all the information about the collinear splitting.

We now explain why V^{coll} can be written as in Eq.(23). Because the collinear splitting $\hat{p} \rightarrow q_1 + q_2 + q_3$ decouples from the rest of the process, V^{coll} is obtained as the sum squared of all possible diagrams that describe a transition of an off-shell parton with momentum \hat{p} into three particles with momenta $q_{1,2,3}$. The propagator of the off-shell parton \hat{p} is included in V^{coll} . In the massless case the matrix $V^{\text{coll}}(n, \hat{p}, q_2, q_3)$ can be written as [13]:

$$V^{\text{coll}} = \left(\frac{\mu_0^2}{\hat{p}^2} \right)^2 \left(\sum_{i=1}^3 A_i \not{q}_i + B \frac{\not{p}}{(pn)} \hat{p}^2 \right). \quad (25)$$

The functions A_i and B are dimensionless functions that depend on the scalar products $(q_i q_j)$. To determine the behavior of the amplitude V^{coll} in the collinear limit, we rescale the transverse momenta:

$$q_{i, \perp} \rightarrow \kappa q_{i, \perp} \quad (26)$$

and consider the limit $\kappa \rightarrow 0$. Since $(q_i q_j) \sim \mathcal{O}(q_\perp^2)$, the functions A_{1-3} and B remain invariant under that rescaling. As follows from Eq.(14), the matrices \not{q}_i transform as: $\not{q}_i \rightarrow z_i \not{p} + \mathcal{O}(\kappa)$. Therefore, after the rescaling Eq.(26), the amplitude V^{coll} becomes:

$$V^{\text{coll}} = \kappa^{-4} \left(\frac{\mu_0^{2\epsilon}}{\hat{p}^2} \right)^2 \left(\sum_{i=1}^3 A_i z_i \right) \not{p} + \mathcal{O}(\kappa^{-3}). \quad (27)$$

Because the collinear phase space Eq.(20) transforms as:

$$d\Phi^{\text{coll}}(q_2, q_3) \rightarrow \kappa^{4-4\epsilon} d\Phi^{\text{coll}}(q_2, q_3), \quad (28)$$

under the rescaling Eq.(26), it follows that in the collinear limit $\kappa \rightarrow 0$ only the first term in Eq.(27) gives non-vanishing contribution after the phase-space integration. This proves that V^{coll} has the form shown in Eq.(23). We can extract the function W from V^{coll} by applying the projection:

$$W = \frac{\text{Tr} [\not{p} V^{\text{coll}}]}{4(pn)}. \quad (29)$$

We now generalize this result to the case when at least one of the final state particles is a quark with mass m . The mass m is considered to be of the order of the transverse momenta of the collinear particles. We follow the same line of reasoning that leads to Eq.(25) allowing, however, for non-vanishing masses in the initial and final states of the collinear splitting process. Eq.(25) generalizes to:

$$V^{\text{coll}} = \left(\frac{\mu_0^{2\epsilon}}{\hat{p}^2 - m_{in}^2} \right)^2 \left(\sum_{i=1}^3 A_i^{(m)} \not{q}_i + B^{(m)} \frac{\not{p}}{(pn)} + Cm \right). \quad (30)$$

In Eq.(30), m_{in} is the mass of the parton that initiates the collinear splitting. The functions $A_i^{(m)}$, $B^{(m)}$ and C are scalar functions of dimension zero, two and zero respectively; they depend on $(q_i q_j)$ and m^2 . These functions possess a regular $m \rightarrow 0$ limit. In the collinear limit, when both the transverse momenta and the mass m are rescaled simultaneously,

$$q_{i,\perp} \rightarrow \kappa q_{i,\perp}, \quad m \rightarrow \kappa m, \quad (31)$$

the scaling properties of the functions $A_i^{(m)}$, $B^{(m)}$ and C coincide with their mass dimension. Therefore, under the rescaling Eq.(31), the amplitude V^{coll} behaves as:

$$V^{\text{coll}} = \kappa^{-4} \left(\frac{\mu_0^{2\epsilon}}{\hat{p}^2 - m_{in}^2} \right)^2 \left(\sum_{i=1}^3 A_i^{(m)} z_i \right) \not{p} + \mathcal{O}(\kappa^{-3}). \quad (32)$$

This result implies that also for the $m \neq 0$ case, the function W is given by Eq.(29). Finally, assembling all the pieces, we find that the function $\tilde{D}(z)$ in Eq.(7), can be written as:

$$\tilde{D}(z) = \frac{1}{z} \int [dq_2; m_2] [dq_3; m_3] \frac{\text{Tr} [\not{p} V^{\text{coll}}(\hat{p}, q_2, q_3, n; m)]}{4(pn)} \delta \left(1 - z - \frac{(nq_2)}{(pn)} - \frac{(nq_3)}{(pn)} \right). \quad (33)$$

Although we have derived Eq.(33) for the one-to-three splitting contribution to $D_a^{\text{ini}}(z, \mu_0/m)$, similar expression is valid when virtual corrections are included. In addition, Eq.(33) can be used to derive the function \tilde{D}^L after the mass m is set to zero everywhere.

We now discuss how to perform phase space integrations in Eq.(33). The approach proposed in [6, 7] requires integration over the transverse momentum up to the scale $\mu_\perp = \mu_0$ for both \tilde{D} and \tilde{D}^L . While this allows a simple calculation of the fragmentation function at $\mathcal{O}(\alpha_s)$, this approach becomes impractical in higher orders of perturbation theory. It is possible to simplify the calculation considerably by realizing that the limit $\mu_\perp \rightarrow \infty$ can be taken when the *difference* of massive and massless functions \tilde{D} is considered. The technical simplification associated with this is twofold. First, all higher order QCD effects in the massless function \tilde{D}^L vanish, because all the integrals that contribute there become scaleless. We obtain:

$$\tilde{D}_{a/b}^L(z, \mu_0, \epsilon) = \delta_{ab} \delta(1 - z). \quad (34)$$

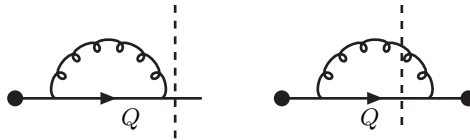


FIG. 1: Diagrams that contribute to perturbative fragmentation of a heavy quark $Q \rightarrow Q + X$ at $\mathcal{O}(\alpha_s)$. The dashed vertical line indicates the intermediate state that has to be considered.

Second, in the massive case, only single-scale integrals have to be computed. Using Eq.(34), we obtain a simple expression for the initial condition of the perturbative fragmentation function:

$$D_a^{\text{ini}}\left(z, \frac{\mu_0}{m}\right) = \sum_b \Gamma_{ab}(z, \mu_0) \otimes \tilde{D}_{b/Q}\left(z, \frac{\mu_0}{m}\right). \quad (35)$$

From this it follows, that $\tilde{D}_{b/Q}$ is the bare fragmentation function for the massive quark, whereas D^{ini} represents its collinear renormalized version.

As we mentioned earlier, there are three contributions to $\tilde{D}_{b/Q}(z, \mu_0, m)$, that have to be considered: double-virtual, real-virtual and double-real. In all these cases the amplitude V^{coll} can be constructed by applying conventional Feynman rules to describe the transition of a parton with momentum \hat{p} to the final state of up to three particles with momenta $q_{1,2,3}$. Virtual corrections should also be included, when appropriate. For each of these three cases, the function W is obtained using the same projector as in Eq.(35). The only unusual feature of the amplitudes that contribute to V^{coll} is that the spinor, that describes the initial state parton, has to be replaced with the propagator of the same parton with the off-shell momentum \hat{p} . V^{coll} is then given by the square of the corresponding matrix element. Standard symmetry factors apply in this case as well. In particular, to evaluate \tilde{D} one has to sum over spins and colors of the final state and to average over colors in the initial state. The ultraviolet renormalization is performed in a standard fashion. One has to renormalize the QCD coupling constant, the quark mass and external quark and gluon fields. Since we work in the light cone gauge, we find it convenient to compute the quark and gluon field renormalization constants by computing diagrams with self-energy insertions to external quark and gluon lines.

Finally, we comment on the double virtual contributions to the fragmentation function. Such contributions describe the one-to-one splitting and are proportional to $\delta(1-z)$. Unfortunately, computing these contributions requires dealing with well-known complications of light-cone gauges. For this reason, we decided to fix the (ϵ -dependent) coefficient of $\delta(1-z)$ using the fermion number conservation sum rule:

$$\int_0^1 dz \left(D_{Q/Q}^{\text{ini}}(z) - D_{\bar{Q}/Q}^{\text{ini}}(z) \right) = 1. \quad (36)$$

We do not encounter, however, any spurious light-cone singularities in the diagrams with one virtual loop. All singularities originating from those diagrams are consistently regulated with dimensional regularization.

To perform integrations in phase-space and loop integrals we proceed as in [15, 16, 17], where further details of the method can be found. The idea is to map all non-trivial phase-space integrals to loop integrals and use standard multiloop methods [18], such as integration-by-parts and recurrence relations, to reduce all the phase-space and loop integrals that have to be evaluated, to a few master integrals. For the reduction to master integrals we use the algorithm [19] implemented in [20]. All algebraic manipulations have been performed using Maple [21] and Form [22]. We now discuss the calculation of the initial condition D^{ini} through $\mathcal{O}(\alpha_s)$ which allows us to illustrate the details of the method by considering a simple example.

IV. D^{ini} AT NLO

In this Section we compute the initial condition for the fragmentation function at NLO through $\mathcal{O}(\epsilon)$. Such terms are needed for the computation of D^{ini} at order $\mathcal{O}(\alpha_s^2)$. The function V^{coll} for $Q \rightarrow Q + g$ splitting is obtained by considering the diagrams shown in Fig.1. To facilitate the comparison with the literature, we express the function W , Eq.(29), through the so-called splitting function P [13]:

$$W = \left(\frac{8\pi\alpha_s\mu_0^{2\epsilon}}{\hat{p}^2 - m^2} \right) P. \quad (37)$$

Introducing auxiliary vector \hat{n} :

$$\frac{n}{(pn)} = (1-z)\hat{n}, \quad (38)$$

and using the projector Eq.(29), we obtain the splitting function:

$$P^{(1)} = C_F \left(2 \frac{(pn)}{(qn)} + (1 - \epsilon) \frac{(qn)}{(pn)} - 2 - m^2 \frac{(pn) - (qn)}{(pq)(pn)} \right). \quad (39)$$

Combining Eqs.(18,38), we derive the real emission contribution to the fragmentation function \tilde{D} :

$$\tilde{D}^{(r)}(z) = \left(\frac{\alpha_s^0}{2\pi} \right) \frac{8\pi^2 \mu_0^{2\epsilon}}{1-z} \int [dq; 0] \frac{P^{(1)}}{(pq)} \delta(1 - (\hat{n}q)). \quad (40)$$

Because of the constraint $\delta(1 - (\hat{n}q))$ in Eq.(40), the splitting function simplifies:

$$P^{(1)} = C_F \left(\frac{2}{1-z} - 1 - z - \epsilon(1-z) - z \frac{m^2}{(pq)} \right). \quad (41)$$

The result for $P^{(1)}$ in Eq.(41) agrees with Ref.[12]. When $P^{(1)}$ is used in Eq.(40) we observe that two integrals have to be evaluated. However, those integrals are not independent; an algebraic relation between them can be found using the method of [15, 16, 17]. As a result, $\tilde{D}^{(r)}(z)$ can be expressed through a single “master” integral:

$$I^{(1)} = \int \frac{d^d q}{(pq)} \delta[q^2] \delta[1 - (\hat{n}q)] = (\pi)^{1-\epsilon} \Gamma(\epsilon) m^{-2\epsilon} (1-z)^{1-2\epsilon}. \quad (42)$$

We finally obtain the real emission contribution to the fragmentation function:

$$\tilde{D}^{(r)}\left(z, \frac{\mu_0}{m}\right) = \left(\frac{\alpha_s^0}{2\pi} \right) C_F \left(\frac{4\pi\mu_0^2}{m^2} \right)^\epsilon \frac{(1-\epsilon)\Gamma(\epsilon)(1+z^2)}{(1-z)^{1+2\epsilon}}, \quad (43)$$

valid to all orders in ϵ . To expand this result in ϵ , we use

$$(1-z)^{-1+a\epsilon} = \frac{\delta(1-z)}{a\epsilon} + \sum_{n \geq 0} \frac{(a\epsilon)^n}{n!} \left[\frac{\ln^n(1-z)}{1-z} \right]_+. \quad (44)$$

Virtual corrections are derived by considering self-energy diagrams in the light-cone gauge. The result reads:

$$\begin{aligned} \tilde{D}^{(v)}\left(z, \frac{\mu_0}{m}\right) &= \left(\frac{\alpha_s^0}{2\pi} \right) S_\epsilon C_F \delta(1-z) \left\{ \frac{1}{\epsilon^2} + \frac{1}{\epsilon} \left[\ln\left(\frac{\mu_0^2}{m^2}\right) + \frac{1}{2} \right] + \frac{1}{2} \ln^2\left(\frac{\mu_0^2}{m^2}\right) + \frac{1}{2} \ln\left(\frac{\mu_0^2}{m^2}\right) + \frac{\pi^2}{12} + 2 \right. \\ &+ \epsilon \left[\frac{1}{6} \ln^3\left(\frac{\mu_0^2}{m^2}\right) + \frac{1}{4} \ln^2\left(\frac{\mu_0^2}{m^2}\right) + \left(\frac{\pi^2}{12} + 2 \right) \ln\left(\frac{\mu_0^2}{m^2}\right) + \frac{\pi^2}{24} - \frac{\zeta(3)}{3} + 4 \right] \left. \right\} + \mathcal{O}(\epsilon^2). \end{aligned} \quad (45)$$

Combining Eqs.(43-45), we arrive at the bare perturbative fragmentation function through $\mathcal{O}(\alpha_s)$:

$$\begin{aligned} \tilde{D}_{Q/Q}\left(z, \frac{\mu_0}{m}\right) &= \delta(1-z) + \left(\frac{\alpha_s^0}{2\pi} \right) S_\epsilon C_F \left\{ \frac{1}{\epsilon} \left[\frac{1+z^2}{1-z} \right]_+ + \left[\frac{1+z^2}{1-z} \left(\ln\left(\frac{\mu_0^2}{m^2}\right) - 2 \ln(1-z) - 1 \right) \right]_+ \right. \\ &+ \epsilon \left[\frac{1+z^2}{1-z} \left(\frac{1}{2} \ln^2\left(\frac{\mu_0^2}{m^2}\right) - \ln\left(\frac{\mu_0^2}{m^2}\right) (2 \ln(1-z) + 1) + 2 \ln^2(1-z) + 2 \ln(1-z) + \frac{\pi^2}{12} \right) \right]_+ \left. \right\} + \mathcal{O}(\epsilon^2). \end{aligned} \quad (46)$$

As expected from the fermion number conservation condition, Eq.(36), the integral of $\tilde{D}_{Q/Q}(z, \mu_0/m)$ over z equals 1 and does not receive any corrections at order $\mathcal{O}(\alpha_s)$. Applying collinear renormalization Eq.(35) and substituting $\alpha_s^0 S_\epsilon \rightarrow \alpha_s$ in Eq.(46), we observe that the $1/\epsilon$ term in Eq.(46) cancels and the remaining terms are not modified. Therefore D^{ini} can be read off from Eq.(46) by simply omitting the $1/\epsilon$ term. The $\mathcal{O}(\epsilon^0)$ part of D^{ini} coincides with the result of Ref.[1], while the $\mathcal{O}(\epsilon)$ part is new.

The gluon fragmentation $g \rightarrow Q + \bar{Q}$ can be treated in a similar way. The real emission contribution reads:

$$\tilde{D}_{g/Q}\left(z, \frac{\mu_0}{m}\right) = \frac{\alpha_s^0}{2\pi} \frac{4(2\pi)^{-1+2\epsilon} \mu_0^{2\epsilon}}{z(1-z)} \int [dq; m] \frac{P_{g/Q}}{\hat{p}^2} \delta(1 - (\hat{n}q)). \quad (47)$$

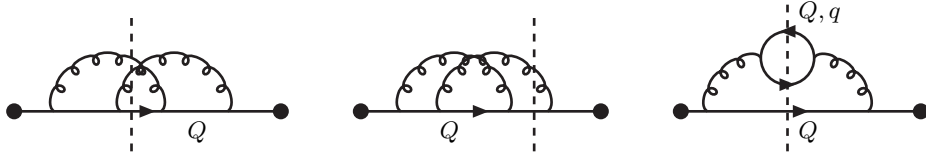


FIG. 2: Examples of diagrams that contribute to perturbative fragmentation of a heavy quark $Q \rightarrow Q + X$ at $\mathcal{O}(\alpha_s^2)$. The dashed vertical line indicates the intermediate state that has to be considered.

Evaluation of the splitting function $P_{g/Q}$ is described in [6]. We derive:

$$P_{g/Q} = T_R \left(1 - 2z \frac{1-z}{1-\epsilon} + \frac{z}{1-\epsilon} \frac{m^2}{(pq)} \right), \quad (48)$$

which agrees with the result in Ref.[12]. There are two integrals of the type:

$$J^{(a)} = \int \frac{d^d q}{(pq)^a} \delta[q^2 - m^2] \delta[1 - (\hat{n}q)] \quad , \quad a = 1, 2, \quad (49)$$

that have to be computed, but only one of them is independent. We obtain:

$$J^{(1)} = (\pi)^{1-\epsilon} \Gamma(\epsilon) m^{-2\epsilon} (1-z). \quad (50)$$

This allows us to derive the gluon-initiated contribution to the initial condition for the perturbative fragmentation function at $\mathcal{O}(\alpha_s)$:

$$\tilde{D}_{g/Q} \left(z, \frac{\mu_0}{m} \right) = \left(\frac{\alpha_s^0}{2\pi} \right) S_\epsilon T_R (z^2 + (1-z)^2) \left\{ \frac{1}{\epsilon} + \ln \left(\frac{\mu_0^2}{m^2} \right) + \epsilon \left[\frac{1}{2} \ln^2 \left(\frac{\mu_0^2}{m^2} \right) + \frac{\pi^2}{12} \right] \right\} + \mathcal{O}(\epsilon^2). \quad (51)$$

The $1/\epsilon$ pole cancels after collinear renormalization and the known result for $\tilde{D}_{g/Q}$ [1] is recovered in the limit $\epsilon \rightarrow 0$. Having explained our method by considering a simple example, we now present the results for D^{ini} through $\mathcal{O}(\alpha_s^2)$.

V. D^{ini} AT NNLO

At NNLO, large number of processes contribute, yet, all of them can be treated using the methods described above. Before we present the results for D^{ini} through $\mathcal{O}(\alpha_s^2)$, we briefly mention some technical details that we find peculiar.

Several sub-processes contribute at $\mathcal{O}(\alpha_s^2)$. It is convenient to split them according to their contributions to various components of D_a^{ini} . The real emission contributions to D_Q^{ini} are $Q \rightarrow Qgg, Qq\bar{q}, QQ\bar{Q}$, while for $D_{\bar{Q}}^{\text{ini}}$ and $D_{q,\bar{q}}^{\text{ini}}$ the real emission sub-processes are $\bar{Q} \rightarrow Q\bar{Q}Q$ and $q(\bar{q}) \rightarrow Qq(\bar{q})\bar{Q}$, respectively. Some of the contributing diagrams are shown on Fig.2.

Because the number of contributing processes is large, there are many possibilities of mass assignments for particles in the final state, relevant for the calculation of D^{ini} . We have to consider all of those cases separately. As we explained in Section III, we require the tree-level splitting amplitudes in the collinear limit when massive quarks are present. Those results are not available in the literature; yet, a useful cross-check of our results is obtained once the limit $m \rightarrow 0$ is taken. In that limit the splitting amplitudes derived in this paper coincide with those in Ref.[13].

We now present the final results for the fermion initiated contributions to the initial condition of the perturbative fragmentation function at order α_s^2 . We give the results for the coefficients $d_a^{(2)}(z, \mu_0/m)$, introduced in Eq.(10). Our results contain polylogarithmic functions up to rank three. These functions are defined through:

$$\text{Li}_n(z) = \int_0^z \frac{\text{Li}_{n-1}(x)}{x} dx, \quad \text{Li}_1(z) = -\ln(1-z), \quad S_{1,2}(z) = \frac{1}{2} \int_0^z \frac{\ln^2(1-x)}{x} dx. \quad (52)$$

We begin with the simplest case of a light (anti)quark-initiated fragmentation process. Through $\mathcal{O}(\alpha_s^2)$, the two contributions coincide:

$$d_q^{(2)} \left(z, \frac{\mu_0}{m} \right) = d_{\bar{q}}^{(2)} \left(z, \frac{\mu_0}{m} \right). \quad (53)$$

We write:

$$d_q^{(2)} = C_F T_R F_q^{(C_F T_R)}, \quad (54)$$

where

$$\begin{aligned} F_q^{(C_F T_R)} = & \left\{ (1+z) \ln(z) + \frac{(1-z)(4z^2+7z+4)}{6z} \right\} L^2 + \left\{ (1+z) \ln^2(z) - \frac{8z^2+27z+15}{3} \ln(z) \right. \\ & \left. - \frac{4(1-z)(14z^2+23z+5)}{9z} \right\} L + \left(2(1+z) \ln(z) + \frac{(1-z)(4z^2+7z+4)}{3z} \right) (\text{Li}_2(z) + \ln(1-z) \ln(z)) \\ & + 4(1+z) \left[\text{Li}_3(z) - \ln(z) \text{Li}_2(z) + \frac{1}{24} \ln^3(z) - \frac{1}{2} \ln(1-z) \ln^2(z) - \zeta(3) \right] - \frac{15+27z+8z^2}{12} \ln^2(z) \\ & + \left(\frac{16}{3} + \frac{56}{3}z + \frac{56}{9}z^2 \right) \ln(z) + \frac{7(1-z)(16+133z+88z^2)}{54z}, \end{aligned} \quad (55)$$

where $L = \ln(\mu_0^2/m^2)$.

Next, we present the heavy antiquark-initiated contribution $d_{\overline{Q}}^{(2)}$. We write:

$$d_{\overline{Q}}^{(2)} = C_F \left(C_F - \frac{C_A}{2} \right) F_{\overline{Q}}^{(C_A, C_F)} + C_F T_R F_{\overline{Q}}^{(C_F T_R)}. \quad (56)$$

The functions $F_{\overline{Q}}^{(C_A, C_F)}$ and $F_{\overline{Q}}^{(C_F T_R)}$ read:

$$\begin{aligned} F_{\overline{Q}}^{(C_A, C_F)} = & \left\{ \frac{1+z^2}{1+z} \left(-4\text{Li}_2(-z) + \ln^2(z) - 4\ln(1+z) \ln(z) - \frac{\pi^2}{3} \right) + 2(1+z) \ln(z) + 4(1-z) \right\} L \\ & + \frac{1+z^2}{1+z} \left(4\text{Li}_3(z) - 2\text{Li}_3(-z) + 12S_{1,2}(-z) + \frac{\ln(z)^3}{2} - 2\ln(z) \text{Li}_2(z) - 2\ln(z) \text{Li}_2(-z) \right. \\ & + 12\ln(1+z) \text{Li}_2(-z) - 3\ln(1+z) \ln^2(z) + 6\ln^2(1+z) \ln(z) - \frac{2\pi^2}{3} \ln(z) - 7\zeta(3) + \pi^2 \ln(1+z) \left. \right) \\ & - \frac{4(12z^2+3z^4+8z^3+1+12z)}{3(1+z)^3} \text{Li}_2(z) + \frac{2(3z^2-1-10z)}{3(1+z)} \text{Li}_2(-z) - \frac{z(-3z+3+z^2+3z^3)}{3(1+z)^3} \ln^2(z) \\ & - \frac{4(12z^2+3z^4+8z^3+1+12z)}{3(1+z)^3} \ln(1-z) \ln(z) + \frac{2(3z^2-1-10z)}{3(1+z)} \ln(1+z) \ln(z) \\ & + \frac{-30z^2+15z^4-9-28z+36z^3}{6(1+z)^3} \ln(z) + \frac{30z^2+28z^3+15z^4+36z+3}{18(1+z)^3} \pi^2 + \frac{45z^3-29z+29z^2-45}{6(1+z)^2}, \end{aligned} \quad (57)$$

and

$$\begin{aligned} F_{\overline{Q}}^{(C_F T_R)} = & \left\{ (1+z) \ln(z) - \frac{4z^2+3z-3}{6} + \frac{2}{3z} \right\} L^2 + \left\{ (1+z) \ln^2(z) - \frac{8z^2+27z+15}{3} \ln(z) \right. \\ & \left. + \frac{56z^2+36z-72}{9} - \frac{20}{9z} \right\} L + (1+z) \left(4\ln(z) \text{Li}_2(z) + 8\ln(z) \text{Li}_2(-z) - 8\text{Li}_3(z) - 16\text{Li}_3(-z) + \frac{1}{6} \ln^3(z) - 4\zeta(3) \right) \\ & + \frac{4(z-1)(z^2+4z+1)}{3z} (\text{Li}_2(z) + 2\text{Li}_2(-z) + \ln(1-z) \ln(z) + 2\ln(1+z) \ln(z)) - \frac{8z^2+27z+15}{12} \ln^2(z) \\ & + \frac{20z^5+351z+48+147z^4+489z^3+713z^2}{9(1+z)^3} \ln(z) - \frac{400z^4-963z+1331z^3-819+499z^2}{54(1+z)^2} + \frac{56}{27z}. \end{aligned} \quad (58)$$

Finally, we present the heavy quark-initiated contribution $d_Q^{(2)}(z, \mu_0/m)$. We write:

$$d_Q^{(2)}\left(z, \frac{\mu_0}{m}\right) = C_F^2 F_Q^{(C_F^2)} + C_A C_F F_Q^{(C_A C_F)} + C_F T_R F_Q^{(C_F T_R)} + C_F T_R n_l F_Q^{(C_F T_R n_l)}, \quad (59)$$

where $n_l = n_f - 1$ is the number of massless flavors. The functions F_Q read:

$$\begin{aligned} F_Q^{(C_F^2)} = & \left\{ \left(\frac{9}{8} - \frac{\pi^2}{3} \right) \delta(1-z) + 4 \left[\frac{\ln(1-z)}{1-z} \right]_+ + 3 \left[\frac{1}{1-z} \right]_+ - \frac{1+3z^2}{2(1-z)} \ln(z) - 2(1+z) \ln(1-z) \right. \\ & \left. - \frac{5+z}{2} \right\} L^2 + \left\{ \left(\frac{27}{8} + \frac{\pi^2}{6} - 2\zeta(3) \right) \delta(1-z) - 12 \left[\frac{\ln^2(1-z)}{1-z} \right]_+ - 14 \left[\frac{\ln(1-z)}{1-z} \right]_+ + \left(1 + \frac{4\pi^2}{3} \right) \left[\frac{1}{1-z} \right]_+ \right. \\ & + (1+z) (2\text{Li}_2(z) - \pi^2) - \frac{3+5z^2}{2(1-z)} \ln^2(z) + \frac{6(1+z^2)}{(1-z)} \ln(1-z) \ln(z) + \frac{(4z^2+4z-1)}{1-z} \ln(z) \\ & + 6(1+z) \ln^2(1-z) + (11+3z) \ln(1-z) + \frac{9z-11}{2} \left. \right\} L + \delta(1-z) \left(\frac{241}{32} + \frac{7\pi^2}{12} - 2\pi^2 \ln(2) - \frac{5\pi^4}{36} + \frac{13\zeta(3)}{2} \right) \\ & + 8 \left[\frac{\ln^3(1-z)}{1-z} \right]_+ + 12 \left[\frac{\ln^2(1-z)}{1-z} \right]_+ - \left(4 + \frac{8\pi^2}{3} \right) \left[\frac{\ln(1-z)}{1-z} \right]_+ - \left(4 + \frac{4\pi^2}{3} - 16\zeta(3) \right) \left[\frac{1}{1-z} \right]_+ \\ & + \frac{1+z^2}{1-z} \left(8\text{Li}_3(-z) - 4\text{Li}_2(-z) \ln(z) + \frac{9}{2} \ln(1-z) \ln^2(z) + \frac{\pi^2}{6} \ln(z) \right) + \frac{2(1+7z^2)}{1-z} \text{Li}_3(z) - \frac{4\zeta(3)}{1-z} \\ & - \frac{7-z^2}{1-z} (\text{Li}_3(1-z) + \text{Li}_2(z) \ln(1-z)) - \frac{8z^2}{1-z} \text{Li}_2(z) \ln(z) - \frac{9z^2+7}{12(1-z)} \ln^3(z) - \frac{17z^2+25}{2(1-z)} \ln^2(1-z) \ln(z) \\ & - 4(z+1) \ln^3(1-z) - \frac{8z(z+1)}{1-z} \text{Li}_2(-z) - \frac{21z^2+22z-22}{3(1-z)} \text{Li}_2(z) + \frac{33z^4-40z^3+3z^2-18z+6}{12(1-z)^3} \ln^2(z) \\ & - \frac{21z^2+46z-13}{3(1-z)} \ln(1-z) \ln(z) - \frac{8z(z+1)}{1-z} \ln(z+1) \ln(z) - 2(z+6) \ln^2(1-z) - \frac{3z^2-5}{2(1-z)} \pi^2 \ln(1-z) \\ & - \frac{63z^4-144z^3+40z^2-32z+9}{6(1-z)^2(z+1)} \ln(z) + \frac{16z-5}{2} \ln(1-z) + \frac{3z^2-10z+6}{6(1-z)} \pi^2 + \frac{21z^2-26z+45}{6(1-z)}, \quad (60) \end{aligned}$$

$$\begin{aligned} F_Q^{(C_A C_F)} = & \left\{ \frac{11}{8} \delta(1-z) + \frac{11}{6} \left[\frac{1}{1-z} \right]_+ - \frac{11}{12} (1+z) \right\} L^2 + \left\{ \delta(1-z) \left(\frac{35}{8} + \frac{11\pi^2}{18} - 3\zeta(3) \right) \right. \\ & \left. - \frac{22}{3} \left[\frac{\ln(1-z)}{1-z} \right]_+ + \left(\frac{34}{9} - \frac{\pi^2}{3} \right) \left[\frac{1}{1-z} \right]_+ + \frac{1+z^2}{2(1-z)} \ln^2(z) + \frac{17+5z^2}{6(1-z)} \ln(z) + \frac{11}{3} (1+z) \ln(1-z) \right. \\ & \left. + \frac{\pi^2}{6} (1+z) + \frac{43-77z}{9} \right\} L + \delta(1-z) \left(\frac{1141}{288} + \frac{41}{54} \pi^2 + \pi^2 \ln(2) + \frac{\pi^4}{36} - \frac{\zeta(3)}{2} \right) + \frac{22}{3} \left[\frac{\ln^2(1-z)}{1-z} \right]_+ \\ & - \left(\frac{68}{9} - \frac{2\pi^2}{3} \right) \left[\frac{\ln(1-z)}{1-z} \right]_+ + \left(\frac{55}{27} + \frac{\pi^2}{3} - 9\zeta(3) \right) \left[\frac{1}{1-z} \right]_+ + \frac{1+z^2}{1-z} (-5\text{Li}_3(z) - 4\text{Li}_3(-z) - \text{Li}_3(1-z) \\ & + \frac{\ln^3(z)}{4} + \text{Li}_2(z)(2\ln(z) + \ln(1-z)) + 2\text{Li}_2(-z) \ln(z) - \ln(1-z) \ln^2(z) + \ln^2(1-z) \ln(z) + \frac{\pi^2}{6} \ln(z)) \\ & - \frac{5z^2-13}{2(1-z)} \zeta(3) + \frac{\pi^2(z^2-3)}{6(1-z)} \ln(1-z) + \frac{33z^2-2z+8}{6(1-z)} \text{Li}_2(z) + \frac{4z(1+z)}{1-z} \text{Li}_2(-z) - \frac{2z^2+4z+7}{3(1-z)} \ln(1-z) \ln(z) \\ & - \frac{13z^4-18z^3+2z^2-2z-11}{24(1-z)^3} \ln^2(z) + \frac{4z(z+1)}{1-z} \ln(z+1) \ln(z) - \frac{(41z+47)}{12} \ln^2(1-z) - \frac{6z^2-4z+3}{12(1-z)} \pi^2 \\ & + \frac{173z-37}{18} \ln(1-z) + \frac{43z^4-159z^3+96z^2-105z+29}{18(1-z)^2(z+1)} \ln(z) + \frac{2z^2-39z-53}{27(1-z)}, \quad (61) \end{aligned}$$

$$\begin{aligned}
F_Q^{(C_F T_R)} = & \left\{ -\frac{1}{2}\delta(1-z) - \frac{2}{3} \left[\frac{1}{1-z} \right]_+ + (1+z)\ln(z) - \frac{4z^2+z-5}{6} + \frac{2}{3z} \right\} L^2 \\
& + \left\{ -\left(\frac{3}{2} + \frac{2\pi^2}{9} \right) \delta(1-z) + \frac{8}{3} \left[\frac{\ln(1-z)}{1-z} \right]_+ - \frac{8}{9} \left[\frac{1}{1-z} \right]_+ + (1+z)\ln^2(z) + \frac{(8z^3+17z^2-12z-17)}{3(1-z)} \ln(z) \right. \\
& - \frac{4}{3}(z+1)\ln(1-z) + \frac{56z^2+52z-80}{9} - \frac{20}{9z} \left. \right\} L + \delta(1-z) \left(\frac{3139}{648} - \frac{\pi^2}{3} + \frac{2}{3}\zeta(3) \right) + \frac{56}{27} \left[\frac{1}{1-z} \right]_+ \\
& + (z+1) \left(-8\text{Li}_3(z) - 16\text{Li}_3(-z) + 4\ln(z)(2\text{Li}_2(-z) + \text{Li}_2(z)) + \frac{\ln^3(z)}{6} - 4\zeta(3) \right) \\
& + \frac{4(z-1)(z^2+4z+1)}{3z} (2\text{Li}_2(-z) + \text{Li}_2(z) + \ln(1-z)\ln(z) + 2\ln(z+1)\ln(z)) + \frac{8z^3+17z^2-12z-17}{12(1-z)} \ln^2(z) \\
& + \frac{20z^9+45z^7+40z^8-339z^6-215z^5-345z^2+921z^4-457z^3+159z+43}{9(z+1)^3(1-z)^4} \ln(z) \\
& + \frac{400z^7+93z^6-1970z^5+963z^4+1396z^3-765z^2-1170z+669}{54(z+1)^2(1-z)^3} + \frac{56}{27z}, \tag{62}
\end{aligned}$$

$$\begin{aligned}
F_Q^{(C_F T_R n_l)} = & \left\{ -\frac{1}{2}\delta(1-z) - \frac{2}{3} \left[\frac{1}{1-z} \right]_+ + \frac{1+z}{3} \right\} L^2 + \left\{ -\left(\frac{3}{2} + \frac{2\pi^2}{9} \right) \delta(1-z) + \frac{8}{3} \left[\frac{\ln(1-z)}{1-z} \right]_+ \right. \\
& - \frac{8}{9} \left[\frac{1}{1-z} \right]_+ - \frac{2(1+z^2)}{3(1-z)} \ln(z) - \frac{4}{3}(1+z)\ln(1-z) + \frac{16z-8}{9} \left. \right\} L - \delta(1-z) \left(\frac{173}{72} + \frac{8}{27}\pi^2 + 2\zeta(3) \right) \\
& - \frac{8}{3} \left[\frac{\ln^2(1-z)}{1-z} \right]_+ + \frac{16}{9} \left[\frac{\ln(1-z)}{1-z} \right]_+ + \frac{4}{27} \left[\frac{1}{1-z} \right]_+ + \frac{1+z^2}{1-z} \left(\frac{4}{3} \ln(1-z)\ln(z) - \frac{\ln^2(z)}{6} \right) \\
& + \frac{4}{3}(z+1)\ln^2(1-z) - \frac{5z^2-12z+5}{9(1-z)} \ln(z) - \frac{16}{9}(2z-1)\ln(1-z) + \frac{19z-23}{27}. \tag{63}
\end{aligned}$$

The results for the functions $d_Q^{(2)}$ and $d_Q^{(2)}$ presented above satisfy the fermion number conservation condition Eq.(36). The two functions are not separately integrable over the interval $0 \leq z \leq 1$ because of the terms $\sim 1/z$; however, all such terms cancel in the difference. The integral of the function $F_Q^{(C_F T_R n_l)}$ over $0 \leq z \leq 1$ vanishes as expected, since $d_Q^{(2)}$ has no terms proportional to n_l .

Our result can be compared with the large- β_0 approximation of Ref. [23]. We have checked that the $\mathcal{O}(\beta_0 \alpha_s^2)$ term in that paper coincides with the n_l -dependent part of our result Eq.(59). Another check of our result is provided by the soft, $z \rightarrow 1$, limit. In such kinematic regime, almost all the energy of the initial parton is transferred to the observed heavy quark in the final state; the energy radiated away in the fragmentation process is small. This leads to large contributions to D^{ini} , of the form $\alpha_s^n \ln^k(1-z)/(1-z)$ with $k \leq 2n-1$, which can be resummed using the soft gluon resummation formalism [6]. When the resummed result in [6] is expanded in powers of α_s through $\mathcal{O}(\alpha_s^2)$, an approximation for $d^{(2)}$, valid for $z \approx 1$, is obtained. We can compare those predictions with the explicit calculation presented in this paper. It is convenient to perform such comparison considering the Mellin moments of $d^{(2)}(z)$. Recall that the Mellin transform is defined as:

$$d_Q^{(2)}(N) = \int_0^1 dz z^{N-1} d_Q^{(2)}(z). \tag{64}$$

A useful summary of Mellin moments is given in Ref.[24]. The soft, $z \rightarrow 1$ limit corresponds to $N \rightarrow \infty$ limit in the Mellin space. In what follows, we present the non-vanishing asymptotics of $d_Q^{(2)}(N)$, for $N \rightarrow \infty$:

$$F_Q^{(C_F)} \rightarrow 2\ln^4(N) + (4L + 8\gamma_E - 4)\ln^3(N) + \left(2L^2 + (12\gamma_E - 7)L + \frac{2}{3}\pi^2 - 2 + 12\gamma_E^2 - 12\gamma_E \right) \ln^2(N)$$

$$\begin{aligned}
& + \left((4\gamma_E - 3)L^2 + \left(\frac{2}{3}\pi^2 - 1 + 12\gamma_E^2 - 14\gamma_E \right) L + \frac{2}{3}(\pi^2 - 6 + 6\gamma_E^2 - 6\gamma_E)(2\gamma_E - 1) \right) \ln(N) \\
& + \frac{1}{8}(4\gamma_E - 3)^2 L^2 + \left(-\pi^2 + \frac{27}{8} + 6\zeta(3) - \gamma_E - 7\gamma_E^2 + \frac{2\gamma_E\pi^2}{3} + 4\gamma_E^3 \right) L + 4\gamma_E - 2\pi^2 \ln(2) - 4\gamma_E^3 \\
& - \frac{3}{2}\zeta(3) + \frac{1}{4}\pi^2 + 2\gamma_E^4 + \frac{2}{3}\pi^2\gamma_E^2 - \frac{2}{3}\pi^2\gamma_E - 2\gamma_E^2 - \frac{11}{180}\pi^4 + \frac{241}{32}, \\
& F_Q^{(C_A C_F)} \rightarrow -\frac{22}{9}\ln^3(N) + \left(-\frac{11}{3}L - \frac{22}{3}\gamma_E - \frac{34}{9} + \frac{\pi^2}{3} \right) \ln^2(N) + \left(-\frac{11}{6}L^2 + \left(-\frac{34}{9} + \frac{\pi^2}{3} - \frac{22\gamma_E}{3} \right) L \right. \\
& \quad \left. - \frac{55}{27} - \frac{14}{9}\pi^2 + 9\zeta(3) - \frac{68}{9}\gamma_E + \frac{2}{3}\pi^2\gamma_E - \frac{22}{3}\gamma_E^2 \right) \ln(N) + \left(-\frac{11\gamma_E}{6} + \frac{11}{8} \right) L^2 + \left(-\frac{11\gamma_E^2}{3} + \frac{35}{8} - 3\zeta(3) \right. \\
& \quad \left. - \frac{34\gamma_E}{9} + \frac{\gamma_E\pi^2}{3} \right) L - \frac{22\gamma_E^3}{9} + \pi^2 \ln(2) + \frac{1141}{288} - \frac{34\gamma_E^2}{9} + \frac{7\pi^2}{54} + \frac{\pi^2\gamma_E^2}{3} + \frac{\pi^4}{12} - \frac{14\pi^2\gamma_E}{9} - \frac{97\zeta(3)}{18} - \frac{55\gamma_E}{27} + 9\zeta(3)\gamma_E, \\
& F_Q^{(C_F T_R)} \rightarrow \frac{4}{3}\ln^2(N)L + \left(\frac{2}{3}L^2 + \frac{8}{9}(3\gamma_E + 1)L - \frac{56}{27} \right) \ln(N) + \left(\frac{2\gamma_E}{3} - \frac{1}{2} \right) L^2 + \left(\frac{4\gamma_E^2}{3} + \frac{8\gamma_E}{9} - \frac{3}{2} \right) L \\
& \quad - \frac{56\gamma_E}{27} + \frac{3139}{648} - \frac{\pi^2}{3} + \frac{2}{3}\zeta(3), \\
& F_Q^{(C_F T_R n_l)} \rightarrow \frac{8}{9}\ln^3(N) + \left(\frac{4}{3}L + \frac{8}{9} + \frac{8}{3}\gamma_E \right) \ln^2(N) + \left(\frac{2}{3}L^2 + \left(\frac{8\gamma_E}{3} + \frac{8}{9} \right) L + \frac{16}{9}\gamma_E - \frac{4}{27} + \frac{8}{3}\gamma_E^2 + \frac{4}{9}\pi^2 \right) \ln(N) \\
& \quad + \left(\frac{2\gamma_E}{3} - \frac{1}{2} \right) L^2 + \left(\frac{4\gamma_E^2}{3} - \frac{3}{2} + \frac{8\gamma_E}{9} \right) L + \frac{8}{9}\gamma_E^3 + \frac{8}{9}\gamma_E^2 + \left(-\frac{4}{27} + \frac{4}{9}\pi^2 \right) \gamma_E - \frac{173}{72} - \frac{4}{27}\pi^2 - \frac{2}{9}\zeta(3). \tag{65}
\end{aligned}$$

Here γ_E is the Euler constant.

Comparing these results with Ref.[6], we find full agreement for all terms $\alpha_s^2(\mu_0) \ln^k(N)$, $k \geq 2$ that were investigated there, provided that we use the matching relation for the coupling constants evolving with n_l and $n_l + 1$ flavors. The results for the subleading $\ln^k(N)$, $k = 0, 1$ terms are new; they can be used to extract the coefficient $H^{(2)}$ (cf. Eq.(70) in [6]) needed to extend the soft gluon resummation for D^{ini} to next-to-next-to-leading logarithmic accuracy.

VI. CONCLUSIONS

In this paper, we derived the initial condition for the heavy quark perturbative fragmentation function through $\mathcal{O}(\alpha_s^2)$. The importance of this result is twofold. First, it enables us to derive energy distributions of heavy quarks produced in hard scattering processes from pure massless calculations. In addition, it can be used to resum large collinear logarithms through NNLL level, using the DGLAP evolution equation.

To derive the initial condition, we make use of the process-independent approach that was recently proposed in [6, 7]. We suggest a simple modification of the original proposal that renders the methods for multi-loop calculations applicable to the calculation of the initial condition of the perturbative fragmentation function.

In the context of QED, an interesting potential application of the initial condition, derived in this paper, is the calculation of the electron energy spectrum in muon decay. Currently, this observable is being very accurately measured in TWIST experiment. The goal of the experiment is to extract Michel parameters [25] from the electron energy spectrum with a relative precision at the level of 10^{-4} . Known results on $\mathcal{O}(\alpha^2 \ln^n(m_\mu/m_e))$, $n = 1, 2$ terms [5, 26] suggest that $\mathcal{O}(\alpha^2)$ corrections without logarithmic enhancement might be important for an unambiguous interpretation of the experimental result. With the initial condition for the fragmentation function at hand, one can obtain the electron energy spectrum in muon decay by computing the energy spectrum for massless electron, removing collinear divergencies by $\overline{\text{MS}}$ renormalization and convoluting decay rate, obtained in this way, with the initial condition for the fragmentation function derived in this paper. This approach simplifies the calculation of the electron energy spectrum in muon decay. Similar methods can be used to extend the results of Ref.[27] on QED corrections to deep-inelastic scattering.

In the context of collider physics, there are many applications for the initial condition of the perturbative heavy quark fragmentation function. First, the B -meson energy spectrum was measured by ALEPH, OPAL and SLD collaborations; this is currently the primary source of information about the b -quark fragmentation function. It has been observed [28] that inclusion of higher order QCD corrections reduces the significance of non-perturbative effects in the bottom quark fragmentation. The knowledge of D^{ini} through $\mathcal{O}(\alpha_s^2)$, permits a reanalysis of B -meson fragmentation with the NNLL accuracy. Another example of potential application is an accurate prediction of the

b -quark energy spectrum in top quark decay. This is currently known to $\mathcal{O}(\alpha_s)$ [29]. The calculation presented in this paper offers the possibility to extend this analysis to $\mathcal{O}(\alpha_s^2)$.

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